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Book Review of Quantum Chemistry, 2nd Edition

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Abstract
This article presents a review of the second edition of *Quantum Chemistry* by D.A. McQuarrie.

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Book & Media Reviews

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Organic Chemistry, 5th Edition

by Marc Loudon

Roberts and Company Publishers: Greenwood Village, CO, 2009. 1472 pp. ISBN: 978-0981519432. $125.

reviewed by James W. Jetter

Marc Loudon's *Organic Chemistry* has a reputation as one of the most widely used textbooks for the first year of college-level organic chemistry. Loudon's classic textbook, now in its fifth edition with a new publisher, brings some improvements over past editions.

Loudon states in the preface of this edition (p XXXI) "an overarching goal of my text is to help students achieve *relational understanding of organic chemistry*" (emphasis in the original). As chemical educators know, complete understanding of organic reaction mechanisms is difficult for many students. The author uses acid−base chemistry in a new approach to provide enhanced insight into reaction mechanisms and problem solving. Chapter 3 contains a nice elucidation of acid−base chemistry and the basic organic chemistry reaction mechanism. This concept is a common theme as the book unfolds.

One great improvement over previous editions is the color enhancement throughout the textbook. For example, many reaction mechanisms are driven home by the use of colored arrows: a red arrow for the base nucleophile and a blue arrow for the leaving group. This use of color-coded arrows in the reaction mechanisms is new to this edition. Not limited to arrows in reaction mechanisms, the color enhancement is also used to add clarity to molecular models, energy diagrams, and to discussions of stereo- and regiochemistry. Another improvement included in this edition is what the author calls tiered topic development, which provides reinforcement of important ideas. For example, Chapter 4 covers the structure and reactivity of alkenes; Chapters 6 and 7 follow up by addressing the application and stereochemistry of alkenes. There are also many examples of how organic chemistry affects our everyday lives. Students could benefit from photographs that accompany many of these real-life applications.

The chapters covering infrared, mass spectrometry, and nuclear magnetic resonance spectroscopy are quite well written, including the problems at the end of each chapter. Chapter 18, "Transition-Metal Catalysis", explains in great detail how transition metals are used as catalysts in forming complexes with various organic compounds. The end of Chapter 18 presents the application of these organometallic catalysts in the Heck, Suzuki, olefin metathesis, and Stille reactions. Other advanced chapters include: Chapter 22, "Enolate Chemistry"; Chapter 23, "Amine Chemistry"; Chapter 24, "Carbohydrate Chemistry"; Chapter 25, "Heterocyclic Chemistry"; Chapter 26, "Peptide Chemistry"; and Chapter 27, "Pericyclic Reactions". As in the fourth edition, Appendix V displays a detailed, summarized list of synthetic methods and their corresponding location within the textbook. Finally, an index completes the very comprehensive fifth edition.

The book has 1672 problem-solving activities, many of which are new to this edition and come directly from relevant literature. The textbook does not include solutions to problems, so the student needs to purchase the *Study Guide and Solutions Manual* for solutions to selected problems. This reviewer did not have access to the *Study Guide and Solutions Manual*, instructor's material, or any online applications that accompany this textbook.

In summary, the renowned reputation of the previous editions of Loudon's *Organic Chemistry* is clearly preserved in this newest edition of the book. If you enjoyed using the fourth edition in your organic chemistry lecture course, then I can recommend this new edition without reservation as a viable replacement for your future use.

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Arrow Pushing in Organic Chemistry: An Easy Approach to Understanding Reaction Mechanisms

by Daniel E. Levy

John Wiley & Sons, Inc.: Hoboken, NJ, 2008. 301 pp. ISBN: 978-20 0470171103 (paper). $42.50.

reviewed by Bridget G. Trogden

"When stuck, draw a dipole!" For teachers who find themselves uttering variations on this statement while teaching organic chemistry, *Arrow Pushing in Organic Chemistry* by Daniel E. Levy will be an important supplement to their course. The text is laid out to introduce fundamental concepts such that the student can learn to rationalize the nature of reactants rather than memorize a list of seemingly unconnected reactions.

The desire to alleviate the memorization game in organic chemistry is a major premise of Levy's book. A few schemes are presented early in Chapter 1 to demonstrate that simply looking at a reaction does not give the reader any insight into the underlying principles at play. The book instead unifies a diverse array of topics by focusing on a central strategy: First, teach the student to identify acids and bases; from there, other concepts fall into place. Electron pairs are described as sources of electron density that drive reactions to occur; just as electricity in a home involves energy flow from regions of higher potential to lower potential, so do molecules need differences in electron density in order to react.

The global view of organic chemistry continues throughout the text. One would expect to see mechanisms presented early in a book that has "arrow pushing" in the title, and this text does not disappoint. Levy describes that bonds are broken and formed through three main types of mechanisms: hemolytic, heterolytic,

and concerted (pericyclic-type) reactions. Students are given problems that introduce electron pushing before any reaction types are even presented, laying the foundation for other concepts. When introducing the all-important concept of the nucleophile, Levy shows the student how to look to multiple competing factors such as basicity, polarizability, sterics, solvent, and electronegativity rather than memorizing a list of hard-and-fast trends that do not hold true in every situation. The reader is always encouraged to think globally and apply a handful of concepts to many different situations.

Much of the success of these strategies relies on the understanding that organic chemistry is traditionally a third-semester chemistry course. Levy's book thus builds upon a general chemistry background. Fundamental explanations are based upon concepts of periodicity and electronegativity that students receive (and typically understand to a reasonable degree) in general chemistry. The Henderson−Hasselbalch equation is reviewed to bring the importance and use of pK_a values to the forefront. When presenting S_N1 reaction mechanisms, Levy spends some time reviewing orbitals and molecular three-dimensional shapes. This is especially noteworthy, as many textbooks present these concepts in earlier chapters and do not discuss them again in detail in later chapters dealing with reactivity. Levy constantly tries to unify the subject of organic chemistry by anchoring new material to that previously learned.

Although the text covers some review material, it also includes many explanations at an earlier juncture or in more depth than what is typically covered in a two-semester organic chemistry textbook. Concepts of induction and resonance are invaluable in determining the stability of a charged species and are given their due early on in the book. Electron-donating groups and electron-withdrawing groups are also presented early, whereas many textbooks do not discuss these fundamental concepts until chapters on electrophilic aromatic substitution. Polarizability and hard−soft base theory are covered to give real information on why certain nucleophiles are better than others, and carbocations are shown to rearrange when they are presented rather than ignored until a later time. The pK_a tables of common functional groups (in Chapter 2 and Appendix 1) provide one-stop comparison shopping for students and professors, the convenience of which is arguably worth the cost of the book! Most notably, the problems presented in each chapter do not just have solutions, they have *explanations*. In fact, almost half of the pages in the book are taken up by these in-depth, comprehensive answers that allow students not only to check themselves, but also to learn from their mistakes.

Arrow Pushing in Organic Chemistry is not meant to replace a traditional textbook, a point that Levy makes clear in the preface. Rather, the text serves as a valuable workbook to counteract student memorization and compartmentalization of organic chemistry material. Review topics are presented in the context of new information, and major concepts are constantly reiterated and highlighted. Levy's book is a great supplemental resource to guide the novice organic chemistry student down the path to a true understanding of the subject.

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Quantum Chemistry, 2nd Edition

by Donald McQuarrie

University Science Books: Sausalito, California, 2007. 690 pp.
ISBN: 978-1891389504 (hardcover). $92.50.

reviewed by Thomas Holme

The modern book-publication cycle is driven largely by economic demands for new editions that mitigate used book markets. For this reason, a lapse of 25 years between editions is uncommon. But this stretch of time may not be surprising in the case of McQuarrie's *Quantum Chemistry*. After all, the intended market for this book is students' first independent quantum chemistry course, although some students may also find it a useful supplement for their junior-level physical chemistry course when it rolls around to quantum. In either case, the market for this type of book is not exactly characterized by its great demand numbers.

The first edition of *Quantum Chemistry* (1983) was a good book that covered the "classic" content of quantum mechanics. Such content includes the historical context, classical wave descriptions, the postulates of quantum chemistry and Schrodinger's equation, particle in a box, harmonic oscillator, rigid rotator, approximation methods, and atoms, molecules, and spectroscopy. The second edition retains this coverage with only modest changes. McQuarrie sometimes includes details in the mathematical treatment of a topic; other times, he leaves the mathematics in end-of-chapter problems. Students who have recently taken advanced mathematics courses will have little difficulty with this style. The expanded number of problems represents a key enhancement in this edition. The problems usually offer good scaffolding that lets students make mathematical connections. However, this strategy may reduce the book's usefulness as a reference for use outside the classroom, as it is hard to predict when ideas will be consigned to an end-of-chapter problem. That said, the instructor can always choose to present the mathematics in lecture or assign it as homework.

Most of the new material in *Quantum Chemistry* appears in the later chapters. The years between 1983 and 2007 saw an explosion in computational chemistry, so the second edition presents the methodology of modern computational quantum mechanics. For example, the final chapter provides a rudimentary discussion of the Hartree−Fock−Roothaan method and additional explanations related to Gaussian basis functions before presenting a sample of computational chemistry software. Making such choices is always risky, but it does not preclude an instructor from using a different computational package. Even with this caveat, the level of material in this section is not on par with previous material in the book. The final content covered is a smattering of brief descriptions of post-Hartree−Fock−Roothaan levels of theory so truncated as to be of modest benefit for students.

In addition to modern computational quantum mechanics, the second edition provides a new series of interchapter sections called MathChapters. The MathChapters include treatments of complex numbers, probability and statistics, vectors, series, spherical coordinates, determinants, matrices, and eigenvalue problems. This feature gives students ample support in understanding the mathematics and physics underlying the book's content. Granted, it would be worrisome if a student taking

a course using this text needed all of these sections, but it is helpful that the topics are available.

As in the first edition, the second edition emphasizes readability. Even within extensive mathematical treatments, McQuarrie does a good job of establishing a narrative flow in the explanations. The first edition was printed entirely in black ink. The second edition has added a brown color to stylistic elements and line graphs. In some places, the added color clarifies the graphical presentation, but it other cases, it seems to add relatively little pedagogical value. An odd aspect of the book's layout is its use of low-resolution screen capture of data. Given the tremendous effort expended in setting the book's mathematical equations, it is anachronistic that so little effort is made to bring these figures to the same level of quality.

My misgivings about some of these details aside, the revisions of McQuarrie's *Quantum Chemistry* are useful. The first edition was always an excellent choice for an introductory course in quantum mechanics; the second edition will not cede that designation. Both editions successfully strike a balance between too much and too little mathematics. Instructors can make pedagogical decisions on where to embellish derivations, knowing that the text offers students a good framework for this material. As a generalized treatment of quantum chemistry, the second edition keeps McQuarrie's text a contender in the textbook market.

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